

Fate Report for Case # P-18-0007

Fate

Summary Statement

Fate P-18-0007-08

Summary FATE: Estimations for

Statement: typical and low weight, MW = 471, C₂₅H₄₂O₈

Liquid with MP < 25 °C

(E)

log K_{ow} = 5.19 (E)

S = 0.81 mg/L at 25 °C (E)

VP < 1.0E-6

torr at 25 °C (E)

BP > 400 °C (E)

H < 1.00E-8 (E)

log K_{oc} =

4.54 (E)

log Fish BCF = 1.72 (52) (E)

log Fish BAF = 1.09 (12) (E)

POTW removal (%) = 90-95 via sorption and biodeg

Time for complete

ultimate aerobic biodeg = wk

Sorption to soils/sediments =

moderate

PBT Potential: P1B1

*CEB FATE: Migration to ground water =

moderate

Bioconcentration factor to be put into E-FAST: 12

PMN

Material:

Overall wastewater treatment removal is 90-95% based on

sorption and biodegradation.

Sorption to sludge is moderate to

strong based on the estimated physical-chemical properties from EPISUITE.

Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE.

Removal by

biodegradation in wastewater treatment is high based on BIOWIN model estimates and analogue data for CASRN 68082-35-9 that showed [REDACTED]

degradation based on COD after 28 days. The analogue achieved 12.5% after

4 days and 61.02% after 14 days, passing the 10-day window criteria and is

considered to be readily biodegradable.

Destruction of the substance

in wastewater treatment is complete based on BIOWIN model estimates and analogue data for CASRN 68082-35-9 that showed [REDACTED] degradation based on

COD after 28 days. The analogue achieved 12.5% after 4 days and 61.02% after 14 days, passing the 10-day window criteria and is considered to be readily biodegradable.

The aerobic aquatic biodegradation half-life

is less than two months based on BIOWIN model estimates and analogue data

for CASRN 68082-35-9 that showed [REDACTED] degradation based on COD after 28

days. The analogue achieved 12.5% after 4 days and 61.02% after 14 days, passing the 10-day window criteria and is considered to be readily biodegradable.

The anaerobic aquatic biodegradation half-life is less

than two months based on the aerobic biodegradation half-life. The

anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is moderate based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater

is moderate based on the estimated physical-chemical properties from EPISUITE.

PMN Material:

Not Persistent (P1) based on the estimated anaerobic biodegradation half-life.

Low Bioaccumulation (B1) based on

BCFBAF model estimates (BCF: 52 and BAF: 12).

Bioconcentration/Bioaccumulation factor to be put into E-Fast: 12.

Fate Placeholder,
Assessor: Legacy
SMILES:

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	C25 H42 O8	

Property	Measured/Calculated Value	EPI
Molecular Wt.:	470.81	
% < 500:		
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					
Boiling Point:			474	EPI, typ.	
BP Pressure:			@760		@760
Vapor Pressure:			<0.000001	EPI, typ.	
Water Solubility:			0.00081	EPI, typ.	
Log P:			5.19		
Log Kow:					
Log Koc:					
Log BCF:					
Henry's Law:					

pH:
pH
Comment:

Fate Analysis

Hydrolysis (t1/2, da):	Volatilization (t1/2)	Volatilization (t1/2)
	- River (hr):	- Lake (da):
Atm Ox Potential (t1/2)OH (hr):	Atm Ox Potential (t1/2)O3 (hr):	Atm Ox Potential (t1/2) Total (hr):
MITI Linear:	MITI NonLinear:	
Biodeg Linear:	Biodeg NonLinear:	

Biodeg Survey	Biodeg Survey
ult:	Prim:
STP (% removal)	STP (% removal)
Total:	Biodeg:
STP (% removal)	STP (% removal)
Ads:	Air:

Rationales

Removal in Wastewater Treatment: Atmospheric Oxidation: Hydrolysis: Photolysis: Aerobic Biodegradation: Anaerobic Biodegradation: Sorption to Soil and Sediment: Migration to Groundwater: Persistence - Air: Persistence - Water: Volatilization from Water: Soil: Sediment: Other: Standard: Bioaccumulation:
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PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1	1	

Exposure-Based Testing

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**Exposure-Based
Testing:**

**Fate Ratings
Removal in WWT/POTW
(Overall):**

**Removal in 90-95
WWT/POTW
(Overall):**

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	2-3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:	2	Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	3	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	3	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio

Comments:

Bio

Comments:

Fate

Comments:

Fate Analog (CAS 68082-35-9):

Comments: OECD 301D(Closed Btl): 69.77%/28d.

Comments/Telephone Log

Artifact	Update/Upload Time